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PROGRESS IN ADVANCED SPRAY COMBUSTION CODE INTEGRATION

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ABSTRACT

A multiyear project to assemble a robust, multiphase spray combustion code is now underway and gradually building up to full speed. The overall effort involves several university and government research teams as well as Rocketdyne. The first part of this paper will give an overview of the respective roles of the different participants involved, the master strategy, the evolutionary milestones, and an assessment of the state-of-the-art of various key components. The second half of this paper will highlight the progress made to-date in extending the baseline Navier-Stokes solver to handle multiphase, multispecies, chemically reactive sub- to supersonic flows. The major hurdles to overcome in order to achieve significant speed ups are delineated and the approaches to overcoming them will be discussed.

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NASA Marshall Space Flight Center

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CFD 93 013-001/D1/PYL

I. GENESIS OF THE IDEA

– – VALUE OF THE FIRST GENERATION EXPERIENCE: ARICC – –

- ARICC STILL REPRESENTS ONE OF THE MOST COMPREHENSIVE PACKAGES OF PHYSICAL MODELS IN ANY CFD CODE
- ARICC DEMONSTRATED THE FEASIBILITY OF FULLY COUPLED THREE-PHASE (DROPLETS, GAS, LIQUID) CFD IN A FINITE VOLUME FORMULATION
- ARICC HIGHLIGHTED THE CRITICALITY OF THE INTER-DISCIPLINARY APPROACH AD THE KEY ROLE OF SEVERAL PHYSICAL PROCESSES IN LIQUID PROPULSION: I.E., ATOMIZATION, EVAPORATION, DENSE SPRAY EFFECTS

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I. GENESIS OF THE IDEA

- - MOTIVATION BEHIND THIS EFFORT - -

TO

ADVANCED STATUS OF MULTI-PHASE SPRAY COMBUSTION MODELING

FROM
A LEVEL OF

TECHNICAL FEASIBILITY

TO
A LEVEL OF

ECONOMIC ATTRACTIVENESS

CF. EXTERNAL FLOW AERODYNAMIC CODES CIRCA 1980.

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II. DETAILS OF THE PLAN

- **ORGANIZATIONAL OBJECTIVE:** **BROADENED SENSE OF OWNERSHIP THROUGH MULTI-PARTY INVOLVEMENT**

- **TECHNICAL OBJECTIVE:** **3–5X REDUCTION IN TURNAROUND TIME THROUGH**
  - MODEST IMPROVEMENT IN COMPUTATIONAL EFFICIENCY
  - LARGE IMPROVEMENTS IN ROBUSTNESS
  - PROVISIONS FOR EVOLVING COMPUTER ARCHITECTURES

- **SCHEDULING OBJECTIVE:** **NEAR-TERM (3 YR), CLEAR-CUT PROJECT COMPLETION THROUGH USE OF**
  - PROVEN LOW RISK METHODOLOGY AS BASE
  - INCORPORATION OF NOVEL ENHANCEMENT FEATURES CURRENTLY BEING DEVELOPED IN OTHER TECHNOLOGY EFFORTS

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APPLICATIONAL OBJECTIVE

OPTIMAL ENGINEER – MODEL INTERFACE (DESIGNER)

HOW TO MAKE CFD MODELS USABLE BY NON-CFD SPECIALISTS?

- EASY PARAMETRIC VARIATION OF HARDWARE GEOMETRY
- EASY VISUALIZATION OF FLOW FIELD AND HEAT LOADING
- EASY DIAGNOSIS OF NUMERICAL PROBLEMS

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MOTIVATION

- **IMPROVED ROBUSTNESS OF NEXT-GENERATION CODE TO BE MEASURED IN TERMS OF**
  - OPERABILITY OVER WIDE RANGE OF DIFFERENT REGIMES
  - COMPUTATIONAL EFFICIENCY FOR BASELINE FLOW PROCESSES
  - INCREASED TOLERANCE OF LOCALLY OR TEMPORARILY STIFF PROCESSES

CODE INTEGRATION STRATEGY

- START WITH
  - PROVEN, PRESSURE-BASED METHODOLOGY OF REACT CODES (BASED ON WORK BY PERIC, 1985)
    - COLLOCATED, PRIMITIVE VARIABLES
    - SEQUENTIAL SOLVER
  - TRANSLPLANT ARICC MULTI-PHASE SUBMODELS
- CLOSELY COORDINATED 2D/3D AND SS/TIME-ACCURATE VERSIONS
- DEVELOP ADVANCED TECHNIQUES FOR OVERCOMING STIFFNESS
  - SOURCE TERM PRE-CONDITIONING
  - GRID ADAPTATION
  - CODING TECHNIQUE FOR PARALLEL COMPUTER ARCHITECTURES

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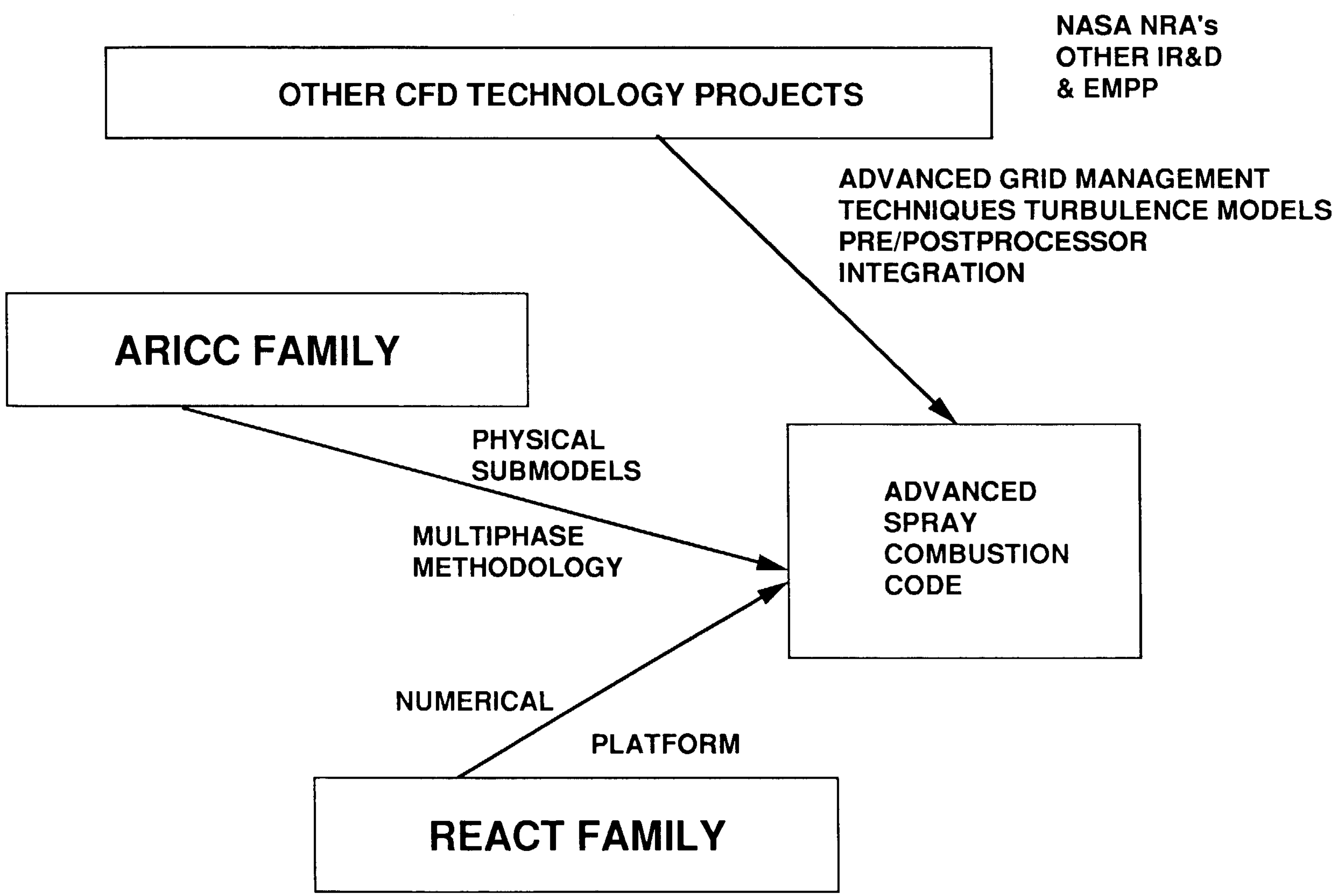
TECHNICAL ROAD MAP FOR ADVANCED SPRAY COMBUSTION CODE



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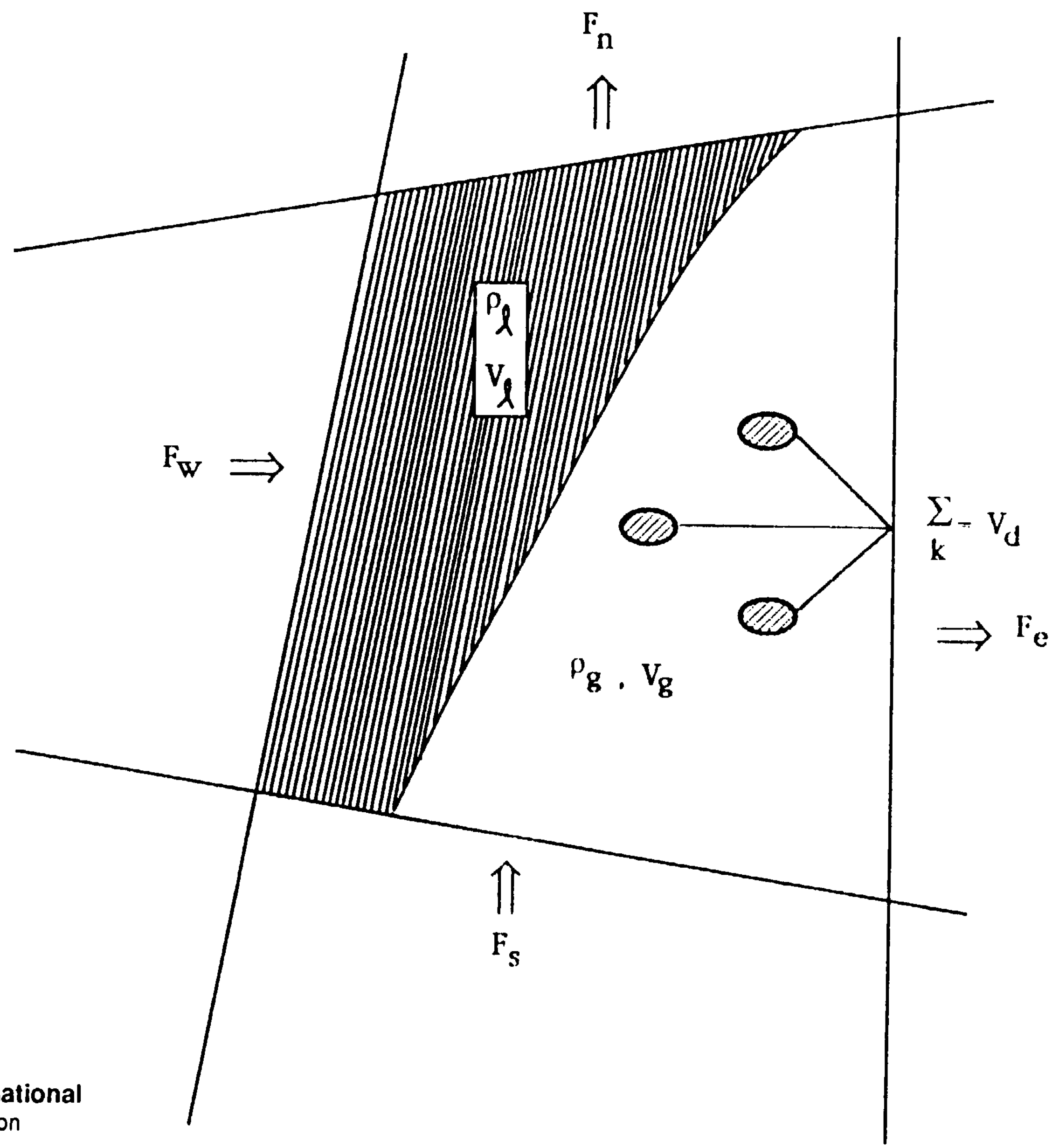
VOF–BASED CELL PARTITIONING IN ASCOMB



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VOLUME-OF-FLUID TWO-PHASE TRACKING SCHEME IMPLEMENTED IN BOTH ARICC AND GALACSY-2D:

<u>G</u>ENERAL <u>AL</u>GORITHM FOR <u>A</u>NALYSIS OF <u>C</u>OMBUSTION <u>SY</u>STEMS

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SUMMARY OF GOVERNING EQUATIONS

mass: $$\frac{\partial\bar{\rho}}{\partial t} + \nabla\bullet(\bar{\rho}\,\mathbf{u}) = \dot{\bar{\rho}}_d \quad \text{where} \quad \bar{\rho} = \mathcal{F}\rho_g + (1-\mathcal{F})\rho_\ell$$

momentum: $$\frac{\partial\bar{\rho}\mathbf{u}}{\partial t} + \nabla\bullet(\bar{\rho}\mathbf{uu}) = -\nabla p - \nabla(\tfrac{2}{3}\bar{\rho}\bar{k}) + \nabla\bullet\underset{\approx}{\sigma} + \mathbf{S} + \bar{\rho}\mathbf{G}$$

internal energy: $$\frac{\partial\bar{\rho}\bar{I}}{\partial t} + \nabla\bullet(\bar{\rho}\bar{I}\mathbf{u}) = -p\nabla\bullet\mathbf{u} - \nabla\mathbf{J} + \bar{\rho}\bar{\varepsilon} + \underset{\text{chemistry}}{\dot{\mathbf{Q}}^c} + \underset{\text{spray}}{\dot{\mathbf{Q}}^s}$$

species m: $$\frac{\partial\bar{\rho}_m}{\partial t} + \nabla\bullet(\rho_m\mathbf{u}\mathcal{F}) = \mathcal{F}\nabla\bullet\left[\rho_g\mathcal{D}\nabla\left(\frac{\rho_m}{\rho_g}\right)\right] + \underset{\text{chemistry}}{\dot{\bar{\rho}}_m^c} + \underset{\text{evaporation}}{\dot{\bar{\rho}}_s\delta_{m,s}}$$

volume fraction: $$\frac{\partial\mathcal{F}}{\partial t} + \nabla\bullet\mathbf{u}\mathcal{F} = \dot{\mathcal{F}}_s = \frac{\text{net gas vol. outflux}}{\text{per unit total vol.}} = \frac{\dot{\bar{\rho}}_s}{\rho_g}$$

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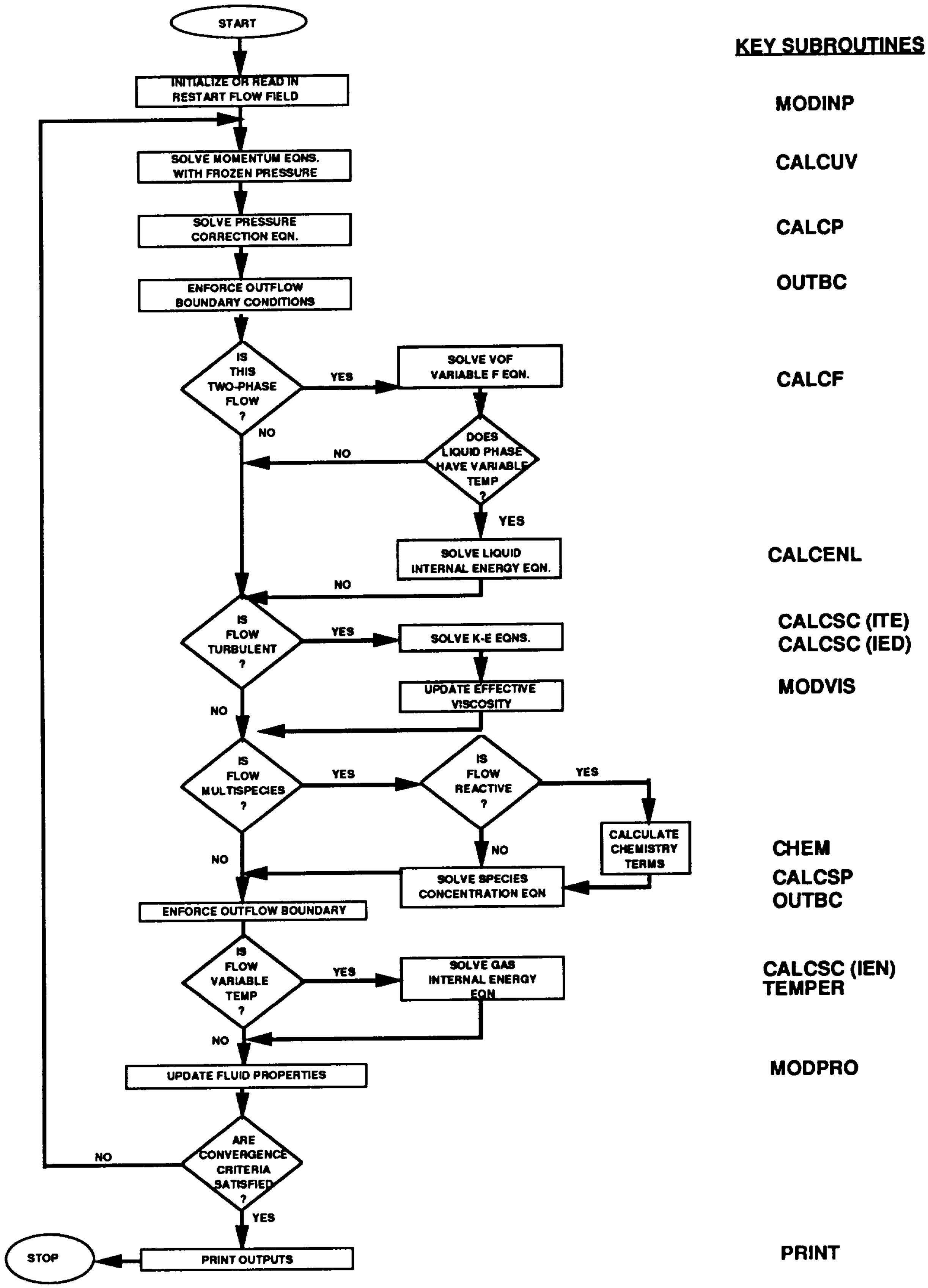
OVERALL FLOW CHART FOR ASCOMB



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SYNOPSIS OF SOLUTION APPROACH

- CAST ALL MATRIX EQUATIONS INTO GENERIC FORM

$$a_P \phi_P = \sum_m a_m \phi_m + C_P$$

WHERE
$$a_P = \sum_m a_m + \dot{\bar{\rho}}_s V_c$$

EXCEPT FOR $\mathscr{F}$-EQUATION, WHERE

$$a_P = \sum_m a_m + \sum_m \dot{V}_m$$

- KEEP COEFFICIENT MATRIX TO 5-DIAGONAL FOR 2D AND 7-DIAGONAL FOR 3D FLOWS BY DOING IMPLICIT DIFFERENCING ONLY FOR CONVECTION AND NORMAL DIFFUSION TERMS.

- SOLVE WITH STONE'S STRONGLY IMPLICIT PROCEDURE

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OBSERVATIONS ON GENERAL FLOW CHARACTERISTICS THAT FORM THE BASIS OF SOLUTION STRATEGY

1. • VELOCITY COMPONENTS STRONGLY COUPLED TO EACH OTHER ONLY BY WAY OF PRESSURE; WEAKLY COUPLED TO TURBULENCE & TEMPERATURE FIELDS

   • HENCE, 2-STEP PRESSURE CORRECTION APPROACH OF "SIMPLE"

   • FLUX UPDATE INCLUDES DENSITY CORRECTION TERM FOR COMPRESSIBLE FLOWS, I.E.,

$$F_{gi} = F^{*}_{gi} + F'_{gi} + \hat{F}_{gi}$$

WHERE

$$F^{*}_{gi} = \mathcal{F}_i\, \rho^{*}_i (u^{*}_1 b^{i}_1 + u^{*}_2 b^{i}_2 + u^{*}_3 b^{i}_3)_i = \mathcal{F}_i\, \rho^{*}_i\, \dot{V}^{*}_i$$

$$F'_{gi} = \mathcal{F}_i\, \rho^{*}_i (u'_1 b^{i}_1 + u'_2 b^{i}_2 + u'_3 b^{i}_3)_i = \mathcal{F}_i\, \rho^{*}_i\, \dot{V}'_i$$

$$\hat{F}_{gi} = \mathcal{F}_i\, \rho'_i (u^{*}_1 b^{i}_1 + u^{*}_2 b^{i}_2 + u^{*}_3 b^{i}_3)_i = \mathcal{F}_i\, \rho'_i\, \dot{V}^{*}_i$$

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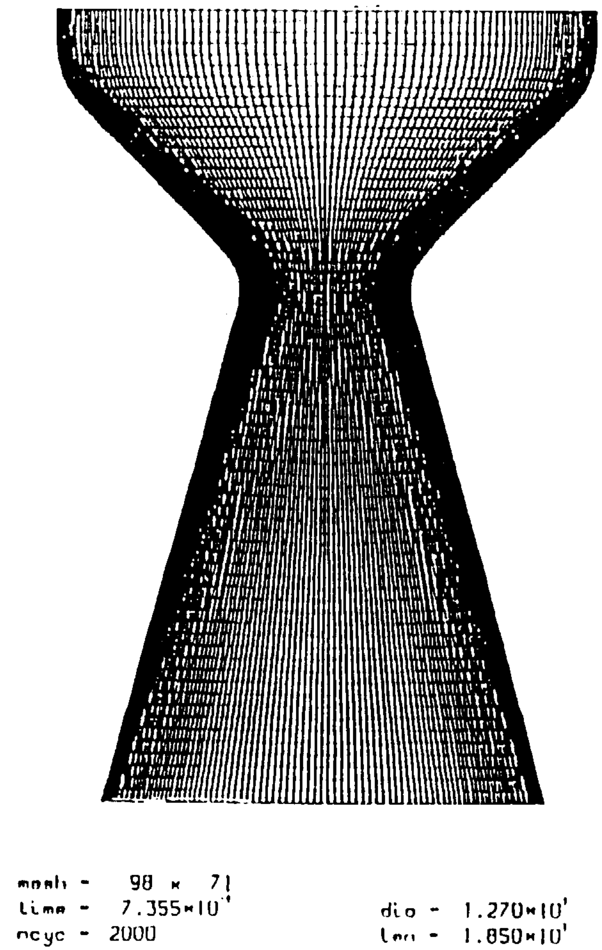
COMPUTATIONAL MESH OF CONICAL NOZZLE TEST CASE



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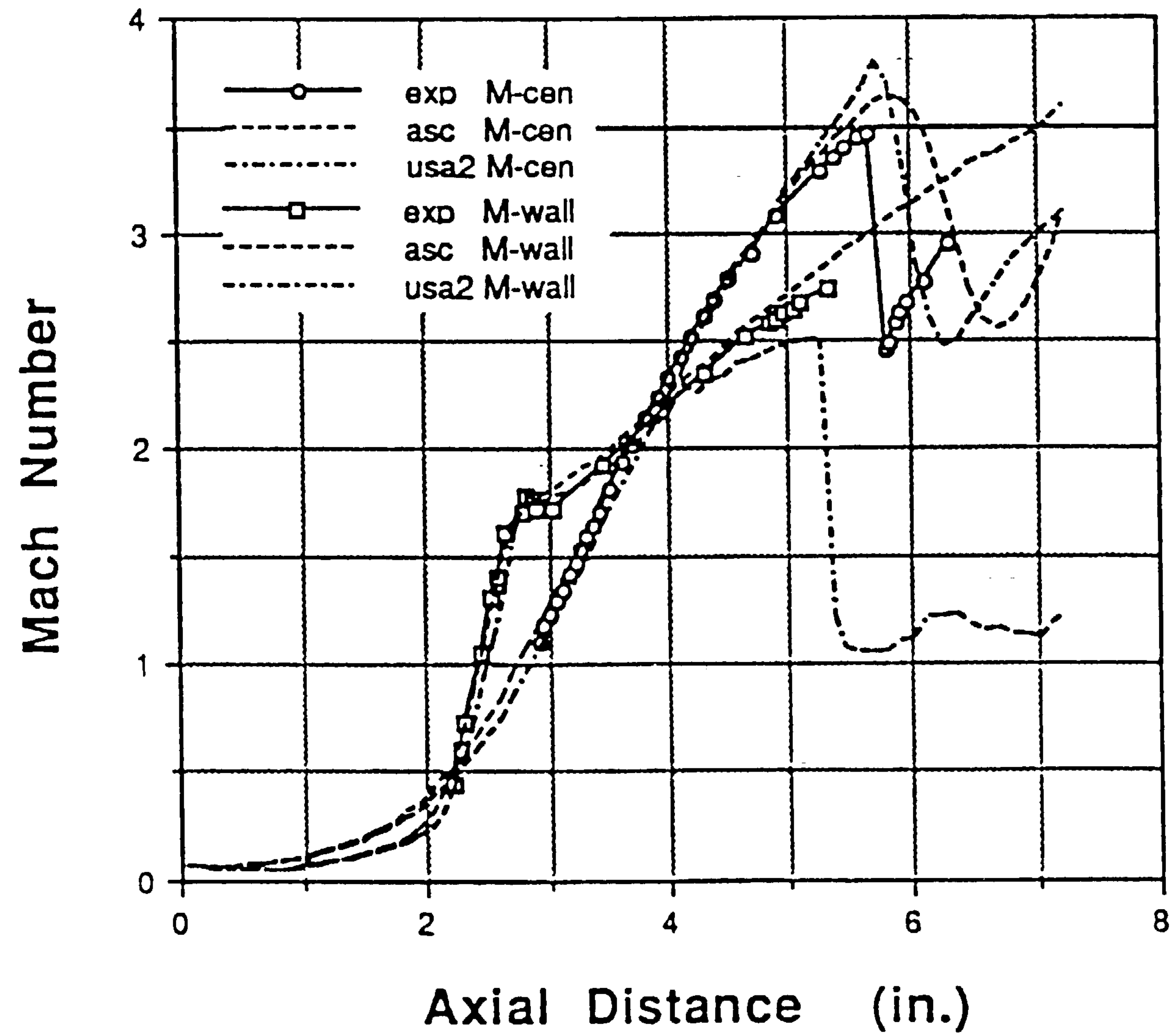
COMPARISON OF CENTERLINE AND WALL MACH NUMBER PROFILES FOR JPL CONICAL NOZZLE



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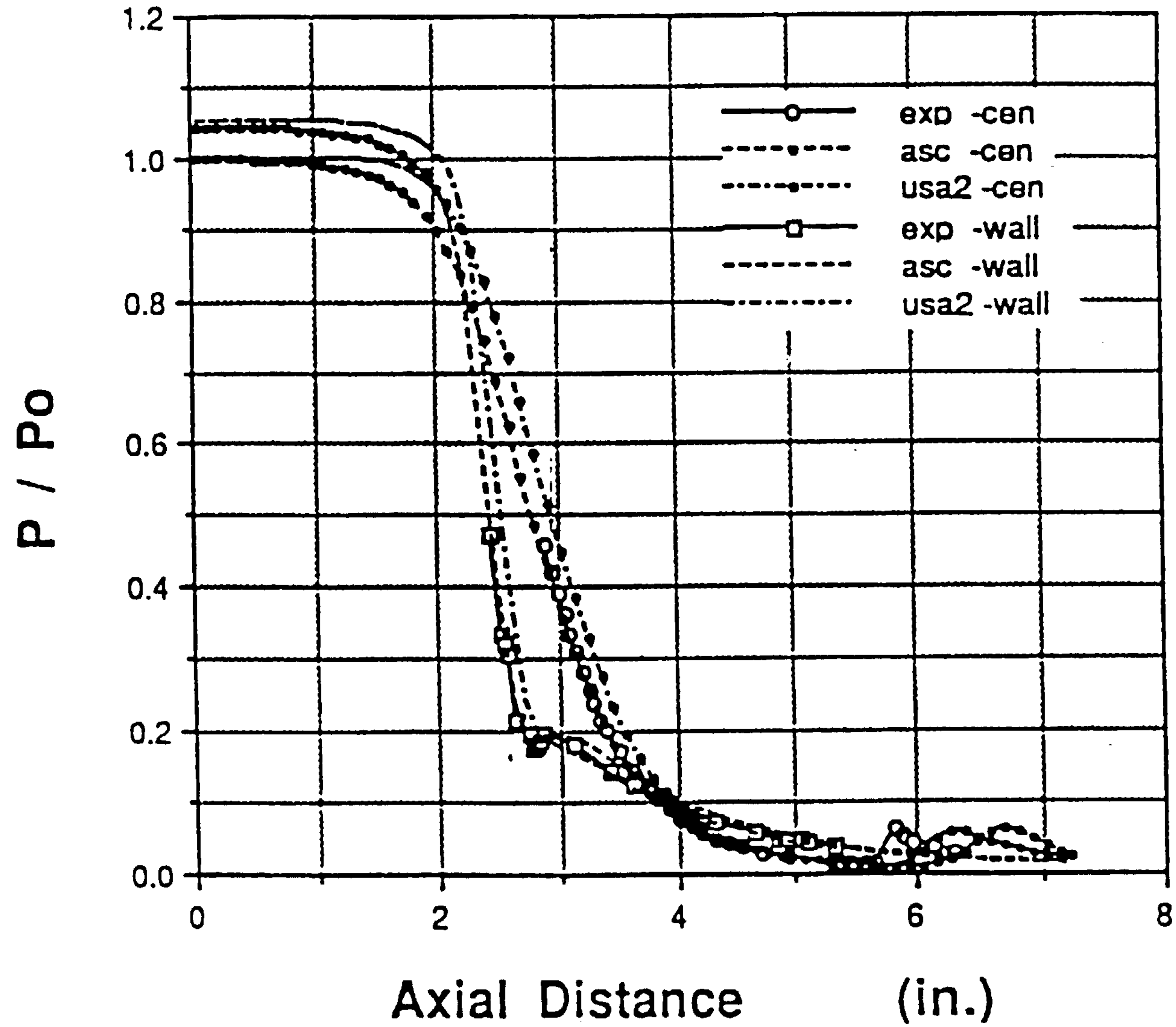
COMPARISON OF CENTERLINE AND WALL PRESSURE PROFILES FOR JPL CONICAL NOZZLE



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CHEMISTRY MODEL UPGRADE

- **SUPER FAST EQUILIBRIUM PACKAGE FOR H/O CHEMISTRY IMPLEMENTED**
- **DIRECT CUBIC SOLVER, 8 SPECIES**
- **FOR EQUILIBRIUM SPECIES, TRANSPORT EQUATIONS FOR ATOMIC TOTAL RATHER THAN FOR INDIVIDUAL COMPOUNDS**

1. $2\,(H_2) + 2(H_2O) + (OH) + (H) + (HO_2) + 2(H_2O_2) = (\hat{H})^\circ$
2. $2\,(O_2) + (H_2O) + (OH) + 2(HO_2) + 2(H_2O_2) + (O) = (\hat{O})^\circ$
3. $1/2\, O_2 + H_2 = H_2O \qquad (H_2O) = (K_{H_2O})\,(H_2)\,(\sqrt{O_2})$
4. $1/2\, H_2 + 1/2 O_2 = OH \qquad (OH) = (K_{OH})\,(\sqrt{H_2})\,(\sqrt{O_2})$
5. $1/2\, H_2 = H \qquad (H) = (K_H)\,(\sqrt{H_2})$
6. $1/2\, H_2 + O_2 = HO_2 \qquad (HO_2) = (K_{HO_2})\,(\sqrt{H_2})\,(O_2)$
7. $H_2 + O_2 = H_2O_2 \qquad (H_2O_2) = (K_{H_2O_2})\,(H_2)\,(O_2)$
8. $1/2\, O_2 = O \qquad (O) = (K_O)\,(\sqrt{O_2})$

- **FOR KINETICS SPECIES, PREVIOUS GENERAL KINETICS MODEL IS RETAINED**

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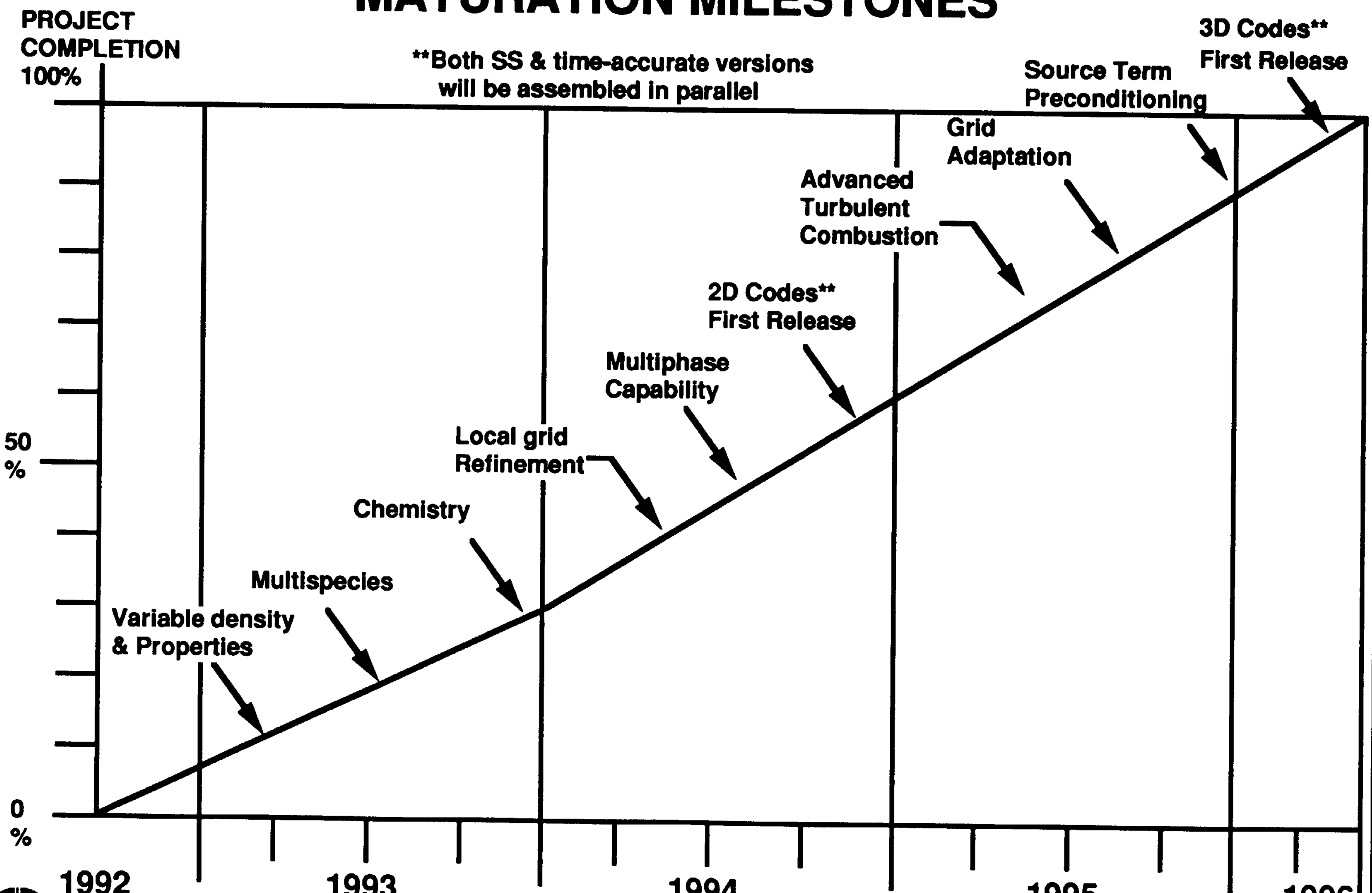
ADVANCED SPRAY COMBUSTION CODE PROGRAM MATURATION MILESTONES



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CONCLUDING REMARKS

- REACT PRESSURE-BASED METHODOLOGY HAS BEEN EXTENDED TO MULTI-PHASE, MULTI-SPECIES, SUPERSONIC FLOWS
- QUANTITATIVE VALIDATION IN PROGRESS
- GOAL OF 10X REDUCTION IN TURNAROUND TIME SEEMS ACHIEVABLE AT LEAST FOR SOME TYPES OF STEADY STATE FLOWS.
- UPCOMING ACTIVITY WILL FOCUS ON
  - LAGRANGIAN SPRAY REPRESENTATION COUPLING SCHEME
  - SOURCE TERM STIFFNESS MITIGATION

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